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Mesoporous perovskite solar cells with Al- and Zn-based metal-organic frameworks

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Abstract. The improvement of lead halide perovskites solar cells (PSC) by hydrophobic metal-organic frameworks (MOF) is one of the promising tools for modern photovoltaic technology to achieve stable and efficient thin-film devices. To show the MOF applicability for PSC, we incorporate two types of MOF: NH_2-MIL-53(Al) and basolite Z1200 in n-i-p mesoporous $MAPbI_3$ based solar cells that can add 2.2% efficiency by increasing main photovoltaic parameters. The simplicity of the proposed MOF's integration allows to use and adopt this approach to incorporate other frameworks for thin-film perovskite devices.

1. Introduction

Perovskite solar cells (PSC) present the new era for thin film photovoltaic technology due to unique properties of active material such as an easily tuneable and direct band gap, high light absorption coefficient and fabrication simplicity. At the same time, perovskite thin films prepared by chemical methods contain many charged defect centers up to $10^{15}/cm^3$ [1] due to the rapid crystal growth and a chemically active surface area.

Metal organic frameworks (MOFs) present three-dimensional crystals constructed of metal ions with a valence (II) higher and organic ligands connecting metal ions. Due to the structuring features MOFs have a high porosity and can be used as a scaffold for material crystallization. Moreover, the choice of organic chains is crucial for thin film perovskite as they can protect a contained material from chemical reactions. The perovskite film crystallization improvement by MOFs and nanoparticles were previously confirmed in a few works [2-7], whereas in our study we compare Basolite Z1200 and NH_2-MIL-53(Al) influence on the main photovoltaic properties of PSCs.

2. Discussion

Commercially available Basolite Z1200 and NH_2-MIL-53(Al) nanocrystals were carried out through a solvothermal route in a DMF–water mixed solvent system with $AlCl_3 \cdot 6H_2O$ and 2-aminoterephthalic acid as the metal source and the organic linker, respectively [8]. Then obtained crystals were dispersed in Ethanol and filtered through PTFE 220 nm pore size filter. Then, each kind of MOF nanocrystals were dropped on the planar mesoporous TiO_2 contained FTO substrates and spin coated at 1000 rpm for 10 s. After that, the $MAPbI_3$ perovskite, SPIRO-MeOTAD and gold layers were deposited by techniques properly described by Furasova [7]. The chemical formulas of NH_2-MIL-53(Al) and Basolite Z1200 compounds are presented in figure 1.

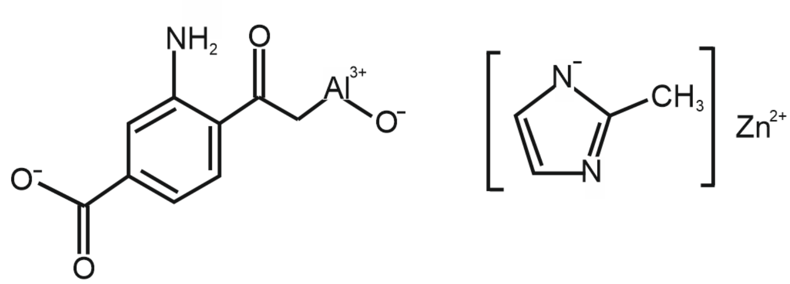

Figure 1. Chemical structure of metal organic frameworks which were used for perovskite solar cells modification. Left: NH_2-MIL-53(Al), right: basolite Z1200.

The thin film perovskite crystal growth can increase mobility for minor and major charges and their lifetime under illumination. As a result, large numbers of charges are able to get through the perovskite-transport layer interband transition, which boost almost all main PSCs parameters. Figure 2 presents J-V curves for the most efficient PSCs: pristine, containing Zn-based and Al-based MOFs. The best reference cell has 13.4% efficiency at short shunt current (J_{SC}) of 18.1 mA/cm^2 and open current voltage (V_{OC}) of 0.951 V, compared to the Basolite Z1200 with 15.4% efficiency with 20.2 mA/cm^2 J_{SC} and 0.967 V V_{OC}. The most efficient cell contains NH2-MIL-53(Al) and achieved 15.8% efficiency at 20.6 mA/cm^2 J_{SC} and 0.955 V V_{OC}.

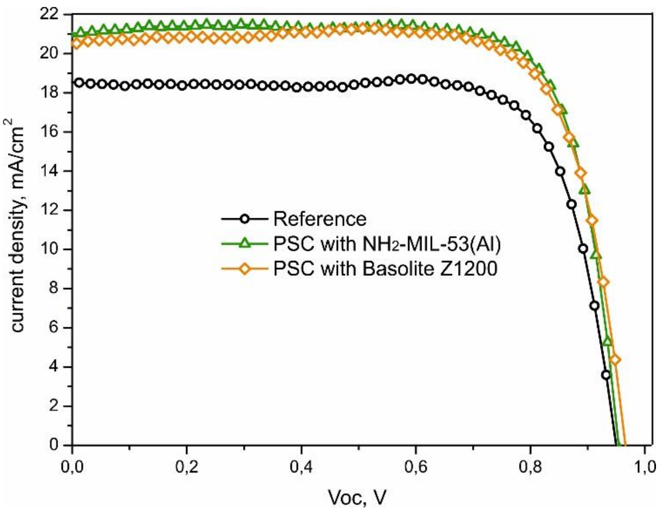

Figure 2. a) JV curves for the best reference (black circles), NH_2-MIL-53(Al) contained device (green triangles) and basolite Z1200 (orange squares) PSCs.

According to the statistical data (Figure 3), the fill factor for all kind of devices remains equal and around 77-79%, whereas the average efficiency improvement relates to the J_{SC} and V_{OC} boosting that confirms perovskite crystallisation improvement by MOF presence.

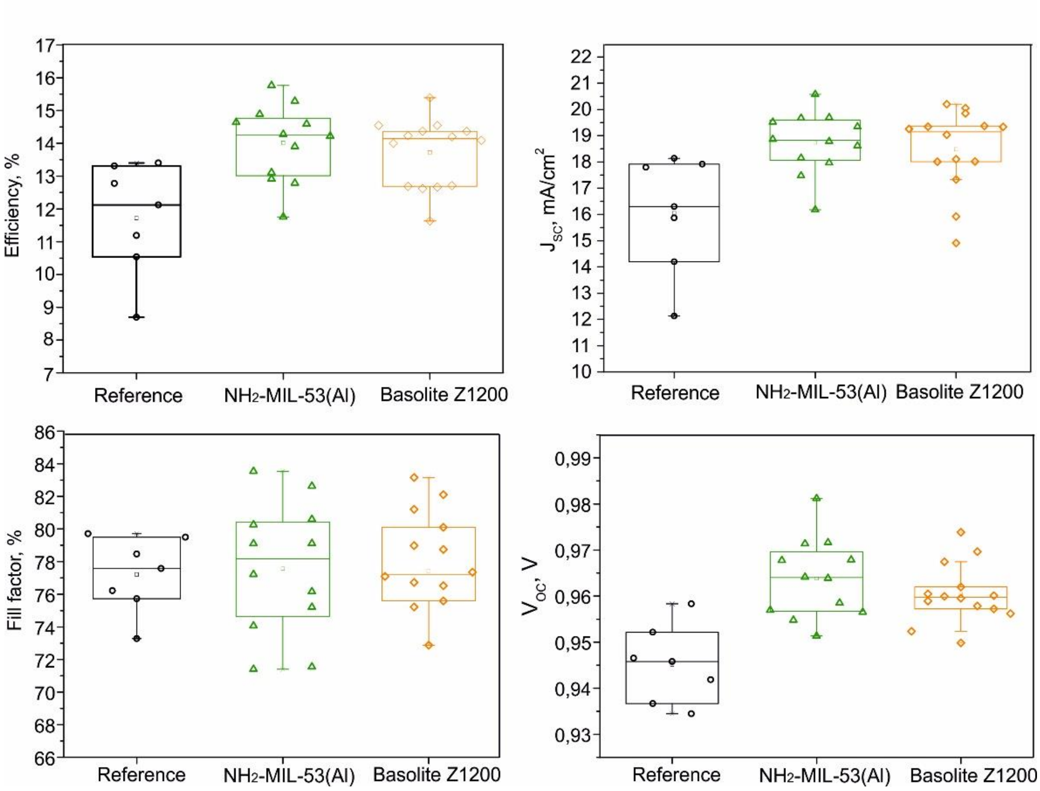

Figure 3. Statistical data for the main photovoltaic parameters (efficiency, short shunt current density - J_{sc}, fill factor, and open current voltage – V_{oc}) of different perovskite devices: black data – reference cells, green - NH_2-MIL-53(Al), orange - basolite Z1200 PSCs.

3. Conclusion

In this work, we have proved that metal-organic frameworks incorporation is a prospective approach to the crystallization improvement of perovskite layer in PSCs. We have demonstrated the high efficiency growth in 2.2% (absolute value) by using NH_2-MIL-53(Al) and in 2% (absolute value) by using basolite Z1200. The proposed PSC's improvement method can be used to prepare perovskite devices with good crystallinity and opens new opportunities for hybrid MOF-perovskite advanced materials.

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